Structural Bioinformatics assignment04

Talha Rehman, Johanna Becher
07 January, 2022

2. Programming exercises

Task 1

Template based modelling was performed on oncogene protein, resulting in five models. The model with the lowest DOPE score of -19026.11914 was selected.

DOPE score is a pairwise atomistic statistical potential which is used to distinguish the good models from the bad ones. The lower the DOPE score, the better is the model. So, it is used to compare models made of single amino acids sequence.

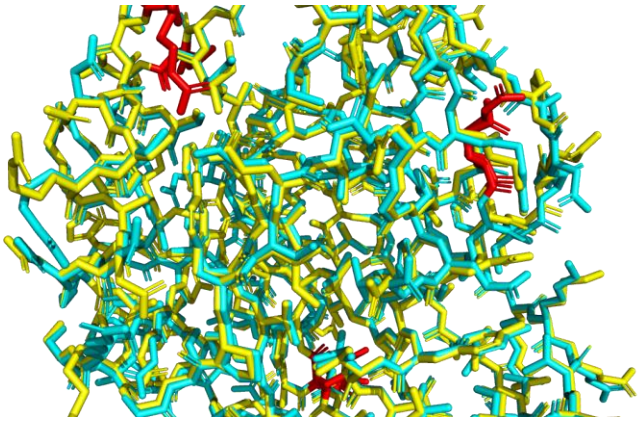
Task 2

Template based modelling was performed, but this time hydrogen atoms were included. The model with the DOPE score of -19111.90625 was selected.

The model which was selected among others had a good score because of hydrogen atoms. Hydrogen bonds are widespread in protein, most of all main chain donors and acceptors have at least one H-bond. H-bonds having side chains describe tertiary and quaternary structure of a protein and contain molecular details of a protein.

Task 3 and 4

(a)



(b)

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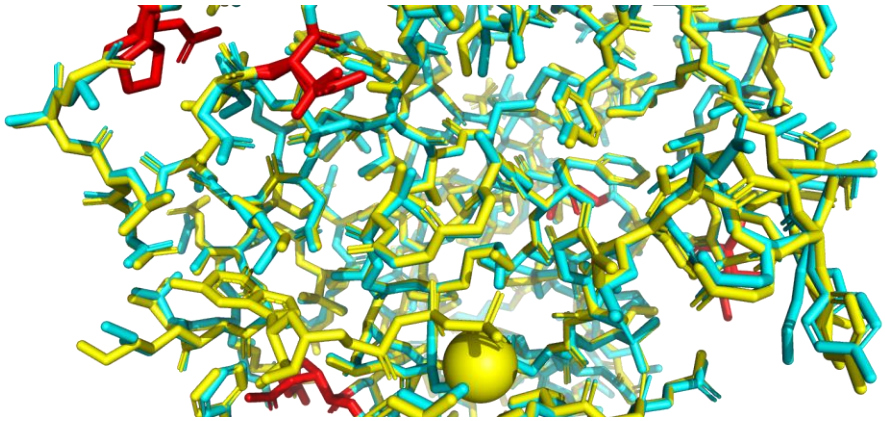

(c)

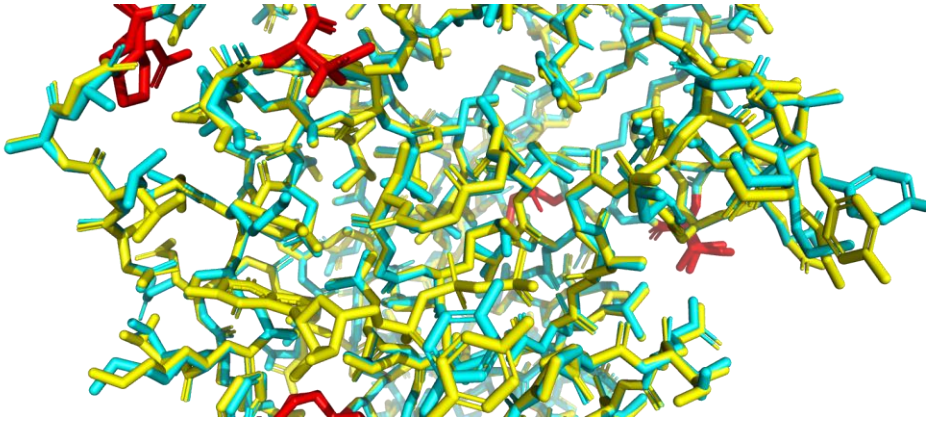

Figure a show the superposition between model from Swiss model and the template protein. It has a root-mean-square deviation RMSD value of 0.420. Since there were less mutations no major changes in the structures were observed apart from the shifting of alpha chains.

Figure b shows the superposition between model obtained by modeller and the template. It has a RMSD value of 0.170. The model with the lowest DOPE score was selected.

Figure c shows the superposition between hydrogen-included model obtained by modeller and the template. It has a root-mean-square deviation RMSD value of 0.168 which is the lowest among the others. RMSD gives the average deviation between the corresponding atoms of two proteins. This concludes that the hydrogen-included model obtained by modeller and the template are the most similar models.